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Extremal First Reformulated Zagreb Index of k-Apex Trees

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Abstract

Consider that G is a finite simple connected graph. The first and second reformulated Zagreb indices of a graph are obtained from the Zagreb indices by using edge degrees instead of vertex degrees, where the degree of an edge is taken as the sum of degrees of vertices incident with the edge minus 2. A graph G is called an apex tree[12] if it has a vertex x such that $G-x$ is a tree. The graph G is k-apex tree for any integer $k \geq 1$ if there exist a subset X of $V(G)$ of cardinality k such that $G-X$ is a tree and for any Y contained in $V(G)$ and cardinality of Y less than k, $G-Y$ is not a tree. In this work we have determined upper and lower bounds of $EM_1(G)$ in k-apex trees.

Key words: Topological index, vertex degree, Zagreb indices, reformulated Zagreb indices, k-apex trees

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1 Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. In chemical graph theory, in 1972 the first and second Zagreb indices were presented by Gutman and Trinajstić to examine the structure-dependency of the total π-electron energy (ϵ) in a paper [8] and were defined as

$$M_1(G) = \sum_{v \in V(G)} d(v)^2 = \sum_{uv \in E(G)} (d(u) + d(v))$$

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

where $d(v)$ is the degree of the vertex v. Applications of Zagreb indices in QSPR were exposed by modeling the structure-boiling point associated with $C_3 - C_8$ alkanes using the CROMRsel method [24]. A large number of work has been done on these two indices. In [7] a history of these descriptors along with their mathematical properties are exhibited. In 2004 Miličević et al.[2] reformulated the Zagreb indices in terms of edge degrees instead of vertex degrees, where the degree of an edge $e = uv$ is described as $d(e) = d(u) + d(v) - 2$. Hence, first and second reformulated Zagreb indices of a graph G are defined as

$$EM_1(G) = \sum_{e \in E(G)} d(e)^2$$

$$EM_2(G) = \sum_{e \sim f} d(e)d(f)$$

where $e \sim f$ means edges e and f are adjacent. Some mathematical properties of reformulated Zagreb indices have been presented in [5]. Ji et al. [22, 23] explored the bounds of these indices for acyclic, unicyclic, bicyclic and tricyclic graphs. All graphs considered in this paper are simple, finite and connected. In a graph G, degree of a vertex v, is the number of edges incident to the vertex v and is denoted by $d(v)$ or $d_G(v)$. A vertex of degree one is called a pendant vertex. The minimum degree of a graph G is the minimum degree of its vertices and is denoted by $\delta(G)$. Neighbour of a vertex u is the set of vertices adjacent to u and is denoted by $N(u)$. We can attain subgraph of a graph by removing edges and vertices. If x is a vertex of G, then $G - x$ is the subgraph obtained from G by deleting the vertex x along with the edges incident to x. In general, if S is any set of vertices in G, we symbolize by $G - S$ the subgraph acquired by deleting the vertices in S and all edges incident to any of them. In graph theory a connected acyclic graph of order n is called a tree and is denoted by T_n. A star is a tree consisting of one vertex adjacent to all other vertices. An n-vertex star is a complete bipartite graph $K(1, n-1)$ and is denoted by S_n [3]. The join of two vertex-disjoint graphs G and K, is the graph $G+K$ with $V(G+K) = V(G) \cup V(K)$ and the edges of $G+K$ are all edges of graphs G and K and edges obtained by joining each vertex of G with each vertex of K. An apex graph is a graph that can be formed planar by removing the single vertex. On the same lines apex trees and k-apex trees were introduced with the name quasi-tree graphs and k-generalized quasi-tree graphs respectively in [1, 4, 12]. An apex tree G is a graph that contains a vertex x such that $G - x$ is a tree, this removing vertex is called an apex vertex. As a tree is always an apex tree therefore a non-trivial apex tree is an apex tree that itself is not a tree. In short 1-apex tree of order n is a non-trivial apex tree of order n and the set of 1-apex trees is expressed as $T_1(n) = T(n)$. A graph G is a k-apex tree of order n if for any integer $k \geq 1$ there exist a subset X of $V(G)$ of cardinality k such that $G - X$ is a tree and for any Y contained in $V(G)$ and cardinality of Y less than k, then $G?Y$ is not a tree. The set of k-apex trees is denoted by $T_k(n)$. In a k-apex tree an edge whose one end is apex vertex and other end is not an apex vertex is called an apex edge. References [11, 18, 19] presents upper and lower bounds on weighted Harary index, Zagreb indices, and Randić index of k-apex trees. Sharp bounds on first and second multiplicative zagreb indices for t-generalized quasi trees has been computed in reference [16]. Zeroth-order general Randić index of k-generalized quasi trees has been calculated in reference [17]

2 Extremal k-Apex Trees for $EM_1(G)$

In the following section we will first compute the upper bounds of the first reformulated Zagreb index for k-apex trees. The following lemma is proved in [22] by using graph operations and we prove it in a very simple way.

Lemma 2.1. If T is a tree of order n, then

$$EM_1(T) \leq (n-1)(n-2)^2$$

and equality holds if and only if $T = S_n$.

Proof: For $e = uv \in E(T)$

$$d(e) = d(u) + d(v) - 2$$

$$d(e) = |N(u)| + |N(v)| - 2$$

As for a tree $N(u) \cap N(v) = \varphi$, therefore

$$deg(e) = |N(u) \cup N(v)| - 2$$

As for a graph of order n, $|N(u) \cup N(v)| \leq n$, therefore

$$d(e) \leq n - 2$$

Hence $EM_1(T)$ is maximum if all edges of T has maximum degree $n-2$. We know there is a unique tree S_n such that $d(e) = n-2$ for all $e \in E(S_n)$ therefore

$$EM_1(T) \leq (n-1)(n-2)^2$$

. ∎

The following Lemma easily follows from definition.

Lemma 2.2. If $u, v \in V(G)$ are not adjacent, then

$$EM_1(G + uv) > EM_1(G)$$

Lemma 2.3. [18] If $G \in T(n)$, $EM_1(G)$ is as large as possible and x is an apex vertex of G, then:
(a) $\delta(G) = 2$ (b) $d(x) = n - 1$

Proof: (a) Suppose that $\delta(G) = 1$ and $y \in V(G)$ is a pendent vertex, then $xy \notin E(G)$ and $G + xy \in T(n)$. By Lemma 2.2 $EM_1(G + xy) > EM_1(G)$, which contradicts our hypothesis. Now we will show that $\delta(G) \leq 2$ for this suppose all vertices have degree greater or equal to three. Now for any vertex $v \in (G)$, each vertex in $G - v$ has degree greater or equal to two, which implies that $G - v$ is not a tree for any $v \in V(G)$. Hence $\delta(G) = 2$.
(b) Let $G \in T(n)$, $EM_1(G)$ is as large as possible and x be an apex vertex of G. Suppose to the contrary that $d(x) < n - 1$, then there is a vertex $y \in V(G)$ such that

$xy \notin E(G)$. Now $G + xy$ is also in $T(n)$ and $EM_1(G + xy) > EM_1(G)$ a contradiction, hence $d(x) = n - 1$. ■

Lemma 2.4. [21] The reformulated first Zegreb index $G_1 + G_2$ is given by

$$\begin{aligned} EM_1(G_1 + G_2) = {} & EM_1(G_1) + EM_1(G_2) + 5|V(G_1)|M_1(G_2) + 5|V(G_2)|M_1(G_1) \\ & + |V(G_1)||V(G_2)|(|V(G_1)| + |V(G_2)| - 2)^2 + 8|E(G_1)||E(G_2)| \\ & + 4(|V(G_1)| + |V(G_2)| - 2)(|V(G_1)||E(G_2)| + |V(G_2)||E(G_1)|) \\ & + 4|V(G_1)|^2|E(G_2)| + 4|V(G_2))|^2|E(G_1)| - 8|V(G_1)||E(G_2)| \\ & - 8|V(G_2)||E(G_1)|. \end{aligned}$$

Theorem 2.5. If $G \in T(n)$ and $n \geq 3$, then

$$EM_1(G) \leq 2(n-2)(n^2-3)$$

and equality holds if and only if $G = k_1 + S_{n-1}$.

Proof: If $G \in T(n)$ and $EM_1(G)$ is as large as possible, then by lemma 2.3 we have $G = K_1 + T_{n-1}$, where T_{n-1} is a tree of order n-1, therefore by using Lemma 2.4 we obtain

$$\begin{aligned} EM_1(G) &= EM_1(K_1 + T_{n-1}) \\ &= EM_1(K_1) + EM_1(T_{n-1}) + 5|V(K_1)|M_1(T_{n-1}) + 5|V(T_{n-1})|M_1(K_1) \\ &\quad + |V(K_1)||V(T_{n-1})|(|V(K_1)| + |V(T_{n-1})| - 2)^2 + 8|E(K_1)||E(T_{n-1})| \\ &\quad + 4(|V(k_1)| + |V(T_{n-1})| - 2)(|V(K_1)||E(T_{n-1})| + |V(T_{n-1})||E(K_1)|) \\ &\quad + 4|V(K_1)|^2|E(T_{n-1})| + 4|V(T_{n-1})|^2|E(K_1)| \\ &\quad - 8|V(K_1)||E(T_{n-1})| - 8|V(T_{n-1})||E(K_1)|. \end{aligned}$$

Using Lemma 2.1, we get

$$EM_1(K_1 + T_{n-1}) \leq 2(n-2)(n^2-3)$$

Lemma 2.1 guaranties that equality holds if and only if $G = K_1 + S_{n-1}$. ■

Theorem 2.6. If $k \geq 2$, $n \geq 2k+1$ and $G \in T_k(n)$, then

$$EM_1(G) \leq (n(k+1) - k(k+3) + (k-1))\,(n+k-2)^2 + \frac{k(k+1)}{2})(2n-4)^2$$

and equality holds if and if $G = K_k + S_{n-k}$.

Proof: We will prove it by induction on k. We have already proved this property for $k = 1$ in theorem 2.5. Now suppose that the result is true for $(k-1)$-apex trees. Let $V_k \subset V(G)$ be the set of k-apex vertices. As $EM_1(G+uv) > EM_1(G)$ for any $uv \notin E(G)$ this implies that V_k forms a complete graph and for any $u \in V_k$, $d(u) = n-1$, so the number m of edges of the graph G is

$$m = \frac{k(k+1)}{2} + (k+1)(n-k-1)$$

Let $x \in V_k$ and $V_{k-1} = V_k - x$ note that $d(x) = n-1$, $G - x$ is a $(k-1)$-apex trees and

$$\begin{aligned}
EM_1(G-x) &= \sum_{uv\in E(G-x)} ((d_G(u)-1)+(d_G(v)-1)-2)^2 \\
&= \sum_{uv\in E(G-x)} (d_G(u)+d_G(v)-4)^2 \\
&= \sum_{uv\in E(G-x)} \left(d_G^2(u)+d_G^2(v)+16+2d_G(u)d_G(v)-8d_G(u)-8d_G(v)\right) \\
&= \sum_{uv\in E(G-x)} \left(d_G^2(u)+d_G^2(v)\right) + 2\sum_{uv\in E(G-x)} d_G(u)d_G(v) \\
&\quad - 8\sum_{uv\in E(G-x)} (d_G(u)+d_G(v)) + 16(m-n+1) \\
&= \sum_{uv\in E(G-x)} \left(d_G^2(u)+d_G^2(v)\right) + \sum_{xu\in E(G)} \left((n-1)^2+d_G^2(u)\right) \\
&\quad - \sum_{xu\in E(G)} \left((n-1)^2+d_G^2(u)\right) + 2\sum_{uv\in E(G-x)} d_G(u)d_G(v) \\
&\quad + 2\sum_{xu\in E(G)} (n-1)d_G(u) - 2\sum_{xu\in E(G)} (n-1)d_G(u) \\
&\quad - 8\sum_{uv\in E(G-x)} (d_G(u)+d_G(v)) - 8\sum_{xu\in E(G)} ((n-1)+d_G(u)) \\
&\quad + 8\sum_{xu\in E(G)} ((n-1)+d_G(u)) + 16(m-n+1) \\
&= \sum_{uv\in E(G)} \left(d_G^2(u)+d_G^2(v)\right) - \sum_{xu\in E(G)} \left((n-1)^2+d_G^2(u)\right) \\
&\quad + 2\sum_{uv\in E(G)} d_G(u)d_G(v) - 2\sum_{xu\in E(G)} (n-1)d_G(u) \\
&\quad - 8\sum_{uv\in E(G)} (d_G(u)+d_G(v)) + 8\sum_{xu\in E(G)} ((n-1)+d_G(u)) \\
&\quad + 16(m-n+1)
\end{aligned}$$

$$
\begin{aligned}
&= \sum_{uv\in E(G)} \left(d_G^2(u) + d_G^2(v)\right) + 2M_2(G) - 8M_1(G) \\
&- \left((n-1)^3 + \sum_{u\in V(G-x)} d_G^2(u)\right) + 8\left((n-1)^2 + \sum_{u\in V(G-x)} d_G(u)\right) \\
&- 2\left((n-1)\sum_{xu\in E(G)} d_G(u)\right) + 16(m-n+1)
\end{aligned}
$$

$$
\begin{aligned}
EM_1(G-x) &= EM_1(G) - 4m - 2M_2(G) + 4M_1(G) + 2M_2(G) - 8M_1(G) \\
&- \left((n-1)^3 + \sum_{u\in V(G-x)} d_G^2(u) + (n-1)^2 - (n-1)^2\right) \\
&+ 8\left((n-1)^2 + \sum_{u\in V(G-x)} d_G(u) + (n-1) - (n-1)\right) \\
&- 2\left((n-1)\left(\sum_{u\in V(G-x)} d_G(u) + (n-1) - (n-1)\right)\right) \\
&+ 16(m-n+1) \\
&= EM_1(G) - 4m - 4M_1(G) \\
&- \left((n-1)^3 + \sum_{u\in V(G)} d_G^2(u) - (n-1)^2\right) \\
&+ 8\left((n-1)^2 + \sum_{u\in V(G)} d_G(u) - (n-1)\right) \\
&- 2\left((n-1)\left(\sum_{u\in V(G)} d_G(u) - (n-1)\right)\right) \\
&+ 16(m-n+1) \\
&= EM_1(G) - 4m - 4M_1(G) - \left((n-1)^3 + M_1(G) - (n-1)^2\right) \\
&+ 8\left((n-1)^2 + (2m-n+1)\right) - 2\left((n-1)(2m-n+1)\right) \\
&+ 16(m-n+1) \\
EM_1(G) &= EM_1(G-x) + 4m + 4M_1(G) + \left((n-1)^3 + M_1(G) - (n-1)^2\right) \\
&- 8\left((n-1)^2 + (2m-n+1)\right) + 2\left((n-1)(2m-n+1)\right) - 16(m-n+1) \\
EM_1(G) &= \left(k(n-1) - (k-1)(k+2) + (k-2)\right)(n+k-4)^2 + \frac{k(k-1)}{2}(2n-6)^2
\end{aligned}
$$

$$
\begin{aligned}
&+4\left(\frac{k(k+1)}{2}+(k+1)(n-k-1)\right)\\
&+4\left((k+1)(n-1)^2+(n-k-1)(k+1)^2\right)\\
&-16\left(\frac{k(k+1)}{2}+k(n-k-2)\right)\\
&+\left((n-1)^2(n+k-1)+(n-k-1)(k+1)^2\right)\\
&-8\left((n-1)(n+k-1)+(n-k-1)(k+1)\right)\\
&+2\left(K(n-1)^2+(k+1)(n-1)(n-k-1)\right)
\end{aligned}
$$

$$
EM_1(G) \quad = (n(k+1)-k(k+3)+(k-1))\,(n+k-2)^2+\frac{k(k+1)}{2}(2n-4)^2
$$

equality holds if and if $G = K_k + S_{n-k}$. ∎

Now we will compute the lower bounds of the first reformulated Zagreb index for k-apex tress.

3 Some graph operations

In this section we will introduce some graph operations[22], which strictly decreases the first reformulated Zagreb index of a graph.

Operation I. Suppose G is a nontrivial connected graph as shown in Fig.1, and v is a given vertex in G. Suppose the graph G has two paths $P : vu_1u_2\ldots u_k$ of length k and $Q : vw_1w_2\ldots w_l$ of length l. If $G' = G - vw_1 + u_kw_1$, we say that G' is obtained from G by Operation I.

Operation II. Let G_0, as shown in Fig.1, be a nontrivial acyclic subgraph of G with $|V(G_0)| = t$, and is attached at u_1 in graph G. Let x and y be two neighbors of u_1 different from vertices in G_0. The graph G_1 as shown in Fig. 2 is obtained from the graph G by changing G_0 into path. If $G' = G_1 - (G_1 - u_1) + u_1u_2 + u_2u_3 + \ldots + u_ty$ we say that G' is obtained from G by Operation II.

In fact, these operations I and II decrease EM_1 of a graph. By the above two graph operations we get the following two result [22].

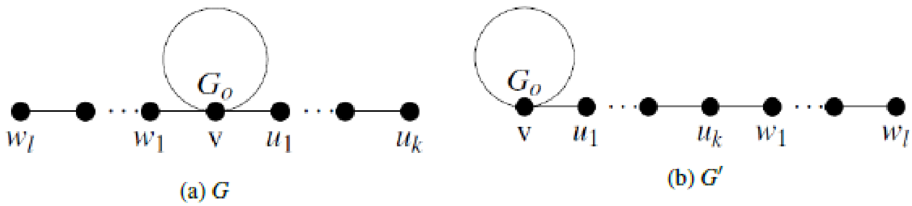

Figure 1: Two graphs G and G' in Operation I

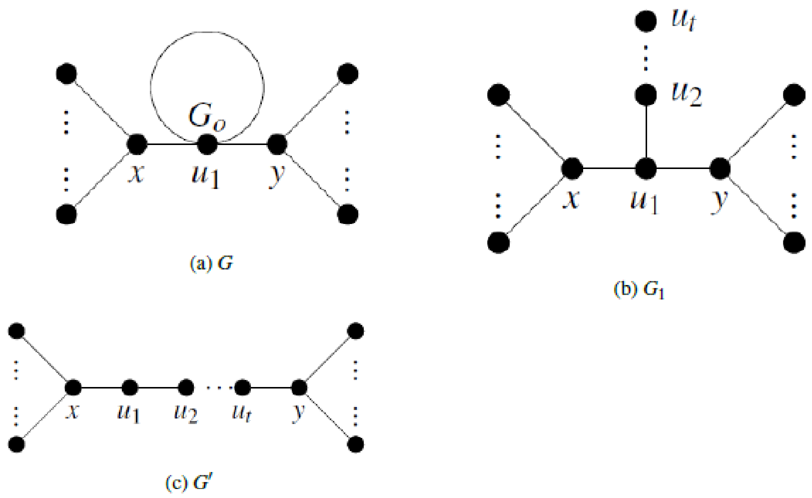

Figure 2: Graphs G,G',G_1 in Operation II

Lemma 3.1. If G' is obtained from G by Operation I as shown in Fig.1, then

$$EM_1(G') < EM_1(G)$$

Lemma 3.2. If G' is obtained from G be the graph Operation II as shown in Fig.2, then we have

$$EM_1(G) > EM_1(G')$$

Theorem 3.3. If $G \in T_k(n)$, $k \geq 1$ and $n \geq 5k - 3$, then

$$EM_1(G) \geq \begin{cases} 4n, & \text{if } k = 1 \\ 4n + 34k - 34, & \text{if } k \geq 2 \end{cases}$$

and equality holds if and only if G has $n - 2k + 2$ vertices of degree 2 and $2k - 2$ vertices of degree 3, and any two vertices of degree 3 are non-adjacent.

Proof: First we prove it for 1-apex trees. Let G be a 1-apex tree and $x \in V(G)$ be an apex vertex. If $d(x) \geq 3$ then for any edge xu, $G - xu$ is still 1-apex tree and $EM_1(G - xu) \leq EM_1(G)$. Hence for minimum $EM_1(G)$, $d(x) = 2$. By operations I and II we get an apex tree G' and it has no pendent edge. The minimum degree of any edge in G' is 2, if we have an apex tree whose each edge has degree two then it will be an apex tree with minimum $EM_1(G)$. A cycle is an apex tree with degree of each vertex two and it is the apex tree with minimum first reformulated Zagreb index.

$$EM_1(G) \geq EM_1(G') = 4n$$

Let G be a k-apex tree ($k \geq 2$). Let $V(G) = \{x_1, x_2, \ldots, x_k, v_1, v_2, \ldots, v_{n-k}\}$ and let $x_1, x_2, \ldots, x_k$ be the apex vertices. If G_1 is the graph obtained from the graph G by deleting edges $x_i x_j$, for $i \neq j$ and $i, j \in \{1, 2, 3, \ldots, k\}$, the G_1 is a k-apex tree and $EM_1(G_1) \leq EM_1(G)$. Suppose that G_2 is the graph obtained from G_1 by deleting edges $v_i x_j$ such that $d_{G_2}(x_j) = 2$ for each $j = 1, 2, \ldots, k$, and G_2 is a k-apex tree then $EM_1(G_2) \leq EM_1(G_1)$. If G_2 has pendent vertices then by operations I and II obtain a k-apex tree G_3 such that $EM_1(G_3) \leq EM_1(G_2)$ and G_3 has no pendent vertex. If all vertices of G_3 are of degree 2, then it is not a k-apex tree ($k \geq 2$). Therefore G_3 has vertices of degree greater than 2. For minimum EM_1, G_3 has vertices of degree 2 and 3

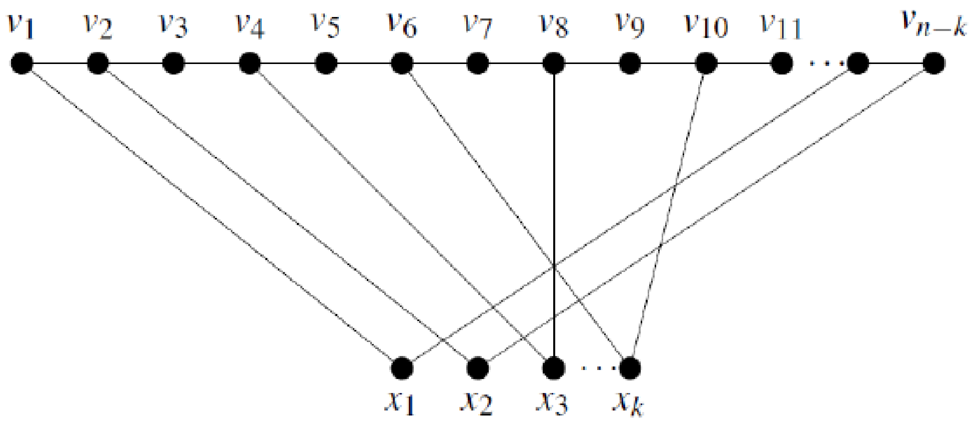

Figure 3: Graph G'

only, and if l is the number of vertices of degree 3, then

$$3l + 2(n - l) = 2n + 2k - 2$$

$$l = 2k - 2$$

Hence EM_1 will be minimum for $n \geq 5k-3$, with $6k-6$ edges of degree 3 and $n-5k+5$ edges of degree 2. One such k-apex tree G' is shown in Fig. 3. Therefor for any k-apex tree G $(k \geq 2)$

$$EM_1(G) \geq (6k - 6)3^2 + (n - 5k + 5)2^2 = 4n - 34k - 34$$

. ∎

4 Conclusion

In this paper we have determined the upper and lower bounds for first Reformulated Zagreb index of k-apex trees. We also characterized the extremal graphs for these indices. It would be interesting to derive similar results for second Reformulated Zagreb index and for other famous indices for example multiplicative Zagreb indices, sum connectivity index, eccentric connectivity index etc. of k-apex trees.

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